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(*
Calculation implemented in Mathematica 6 by Frank Scheffold (Frank.Scheffold@unifr.ch),
University of Fribourg (CH) and University of California Los Angeles (USA),
January-March 2009 based on
  "Measurable Structure Factor of a Multi-Species Polydisperse Percus-Yevick Fluid
    with Schultz distributed Paramters, M.Ginoza and M. Yasutomi, Journal
    of the Physical Society of Japan, 68, 1999, 2292-2297 - MONOCOMPONENENT
    CALCULATION. Default values correspond to Figure 1c in the current JPCM
    article  (particle size in micrometers, wavenumber q in inverse micrometers)
    *)
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$D\sigma := 0.044;\ \eta := 0.77;\ \sigma := 0.135;\ \Delta := 1 - \eta;\ t := \text{Abs}[1/D\sigma] - 1;\ \text{poly} := 1/\sqrt{t+1};$

(*poly is the polydispersity index, σ is the mean particle diameter,
η is the volume fraction of hard spheres*)

poly

$$t0 := 1;\ t1 := 1;\ t2 := \frac{(t+2)!}{t! * (t+1)^2};\ t3 := \frac{(t+3)!}{t! * (t+1)^3};$$

$$\rho := \frac{6}{t3} * \frac{\eta}{\pi * \sigma^3};\ \xi 0 := \rho;\ \xi 1 := \rho * \sigma;\ \xi 2 := \rho * \sigma^2;\ \xi 3 := \rho * \sigma^3;\ F0 := \rho;$$

$$f0[x\_] := t0 * \left(1 + \frac{x}{t+1}\right)^{-(t+1)};$$

$$f1[x\_] := t1 * \left(1 + \frac{x}{t+1}\right)^{-(t+1+1)};$$

$$f2[x\_] := t2 * \left(1 + \frac{x}{t+1}\right)^{-(t+2+1)};$$

$$fa[x\_] := \frac{1}{x^3} * \left(1 - \frac{x}{2} - f0[x] - \frac{x}{2} f1[x]\right);$$

$$fb[x\_] := \frac{1}{x^3} * \left(1 - \frac{x}{2} * t2 - f1[x] - \frac{x}{2} * f2[x]\right);$$

$$fc[x\_] := \frac{1}{x^2} * (1 - x - f0[x]);$$

$$fd[x\_] := \frac{1}{x^2} * (1 - x * t2 - f1[x]);$$

$$F11[x\_] := \frac{2 * \pi * \rho * \sigma^3}{\Delta} * fa[x];$$

$$F21[x\_] := \sigma * \frac{2 * \pi * \rho * \sigma^3}{\Delta} * fb[x];$$

$$F12[x\_] := \frac{1}{\sigma} * \left(\left(\frac{\pi}{\Delta}\right)^2 * \rho * \xi 2 * \sigma^4 * fa[x] + \frac{\pi * \rho * \sigma^3}{\Delta} * fc[x]\right);$$

$$F22[x\_] := \left(\frac{\pi}{\Delta}\right)^2 * \rho * \xi 2 * \sigma^4 * fb[x] + \frac{\pi * \rho * \sigma^3}{\Delta} * fd[x];$$

$$FF11[s\_] := 1 - F11[s * \sigma];$$
$$FF12[s\_] := -F12[s * \sigma];$$
$$FF21[s\_] := -F21[s * \sigma];$$
$$FF22[s\_] := 1 - F22[s * \sigma];$$

$$G11[s\_] := \frac{FF22[s]}{FF11[s] * FF22[s] - FF12[s] * FF21[s]};$$

$$G12[s\_] := \frac{-FF12[s]}{FF11[s] * FF22[s] - FF12[s] * FF21[s]};$$

$$G21[s\_] := \frac{-FF21[s]}{FF11[s] * FF22[s] - FF12[s] * FF21[s]};$$

$$G22[s\_] := \frac{FF11[s]}{FF11[s] * FF22[s] - FF12[s] * FF21[s]};$$

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I0[s_] := -9/2 (2/s)^6 * F0^2 (1 - 1/2 (f0[-s*σ] + f0[s*σ]) +
      (s*σ)/2 (f1[-s*σ] - f1[s*σ]) - (s^2 σ^2)/8 (f2[-s*σ] + f2[s*σ] + 2*t2));
Iα1[s_] := 24/s^3 F0 (-1/2 (1 - f0[s*σ]) + (s*σ)/4 (1 + f1[s*σ]));
Iα2[s_] := 24/s^3 F0 (-σ/2 (1 - f1[s*σ]) + (s*σ^2)/4 (t2 + f2[s*σ]));
Iw1[s_] := (2 π*ρ)/(Δ*s^3) (Iα1[s] + s/2 Iα2[s]);
Iw2[s_] := (π*ρ)/(Δ*s^2) (1 + (π*ξ2)/(Δ*s)) Iα1[s] + (π^2*ξ2*ρ)/(2*Δ^2*s^2) Iα2[s];

h2[q_] :=
  Iw1[Sqrt[-1]*q]*G11[Sqrt[-1]*q]*(Iα1[Sqrt[-1]*q])/(I0[Sqrt[-1]*q]) + Iw1[Sqrt[-1]*q]*G12[Sqrt[-1]*q]*(Iα2[Sqrt[-1]*q])/(I0[Sqrt[-1]*q]) +
   Iw2[Sqrt[-1]*q]*G21[Sqrt[-1]*q]*(Iα1[Sqrt[-1]*q])/(I0[Sqrt[-1]*q]) + Iw2[Sqrt[-1]*q]*G22[Sqrt[-1]*q]*(Iα2[Sqrt[-1]*q])/(I0[Sqrt[-1]*q]);
SM[q_] := 1 - 2*Re[h2[q]];


(*Monodisperse Percus Yevik - for comparison

   a:=(1+2*η)^2/(1-η)^4;b:=-3/2 η(η+2)^2/(1-η)^4;
f[u_]:=1+24*η/u^3 (a(Sin[u]-u*Cos[u]) +
     b((2/u^2-1)u*Cos[u]+2Sin[u]-2/u)+η*a/2*(24/u^3+4(1-6/u^2)Sin[u]-(1-12/u^2+24/u^4)u*Cos[u]));
SPY[q_]:=1/f[q*σ]*)


(*Data and Plots*)

(*us2=Table[{i,SPY[i]},{i,8,200,.2}];
ListPlot[{us2},PlotRange→ {0,1.5}]*)

us = Table[{i, SM[i]}, {i, 8, 200, .2}];
ListPlot[{us}, PlotRange→ {0, 1.5}]

(*Export Data to File*)
(*Export["Documents/PY/temp",us3,"csv"]*)

0.209762
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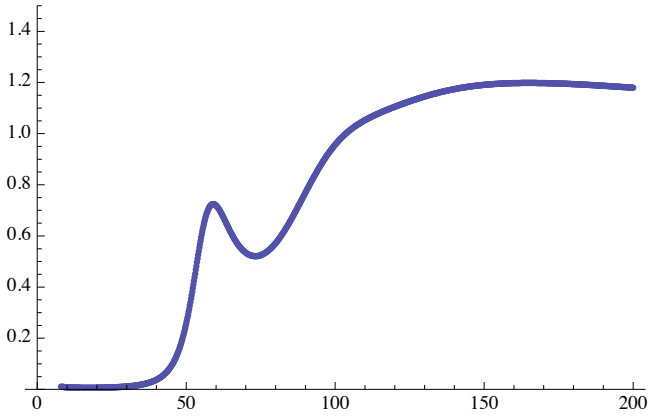
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
50
100
150
200